Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 8.95

Global applicability domain: Inside

Local applicability domain index: 9.85e-01

Confidence level: 8.59e-01

Nearest Neighbors from the Training Set

Image not found 2,3,7-Trichlorodibenzo-p-dioxin **Measured:** 9.14 **Predicted:** 8.95	Image not found 1,2,3,5,7-Pentachloronaphthalene **Measured:** 8.82 **Predicted:** 8.95	Image not found 1,2,3,5,8-Pentachloronaphthalene **Measured:** 9.10 **Predicted:** 8.95
Image not found Pyrene **Measured:** 8.80 **Predicted:** 8.87	Image not found Fluoranthene **Measured:** 8.88 **Predicted:** 8.87	